



## wwPDB EM Validation Summary Report ⓘ

Jun 11, 2024 – 02:52 PM JST

PDB ID : 7VBB  
EMDB ID : EMD-31877  
Title : Structure of the post state human RNA Polymerase I Elongation Complex  
Authors : Zhao, D.; Liu, W.; Chen, K.; Yang, H.; Xu, Y.  
Deposited on : 2021-08-31  
Resolution : 2.81 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

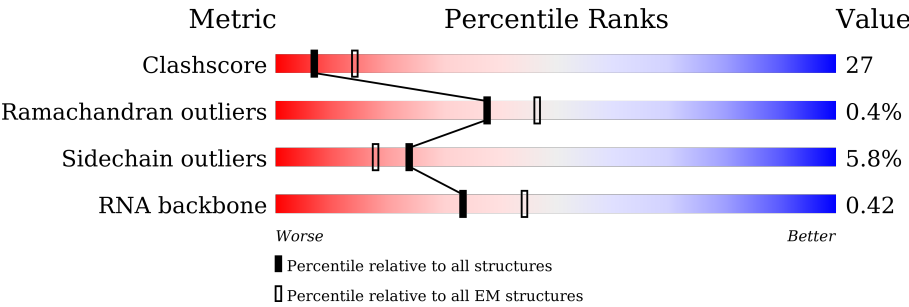
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1719	<div> <div>28%</div> <div>44%</div> <div>39%</div> <div>14%</div> </div>
2	B	1135	<div> <div>12%</div> <div>50%</div> <div>46%</div> <div>..</div> </div>
3	C	346	<div> <div>25%</div> <div>55%</div> <div>39%</div> <div>..</div> </div>
4	E	210	<div> <div>35%</div> <div>47%</div> <div>48%</div> <div>5%</div> </div>
5	F	127	<div> <div>17%</div> <div>42%</div> <div>18%</div> <div>40%</div> </div>
6	H	150	<div> <div>26%</div> <div>55%</div> <div>42%</div> <div>..</div> </div>
7	I	126	<div> <div>41%</div> <div>20%</div> <div>23%</div> <div>..</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
8	J	67	
9	K	133	
10	L	58	
11	N	510	
12	G	338	
13	M	419	
14	R	8	
15	T	25	
16	U	14	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1473	Total	C	N	O	S	0	0
			11749	7474	2063	2134	78		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1123	Total	C	N	O	S	0	0
			8912	5710	1517	1614	71		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	337	Total	C	N	O	S	0	0
			2697	1701	480	505	11		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	199	Total	C	N	O	S	0	0
			1641	1042	286	305	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	146	Total	C	N	O	S	0	0
			1176	744	192	235	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	60	Total	C	N	O	S	0	0
			447	277	76	89	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	108	Total	C	N	O	S	0	0
			863	535	156	165	7		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	45	Total	C	N	O	S	0	0
			379	236	73	64	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1105	698	198	204	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	157	Total	C	N	O	S	0	0
			1229	775	215	232	7		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			867	539	159	163	6		

- Molecule 14 is a RNA chain called RNA (5'-R(P\*UP\*GP\*CP\*UP\*GP\*AP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	8	Total	C	N	O	P	0	0
			168	75	27	58	8		

- Molecule 15 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	25	Total	C	N	O	P	0	0
			514	243	105	142	24		

- Molecule 16 is a DNA chain called DNA (5'-D(\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*GP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	14	Total	C	N	O	P	0	0
			281	135	48	85	13		

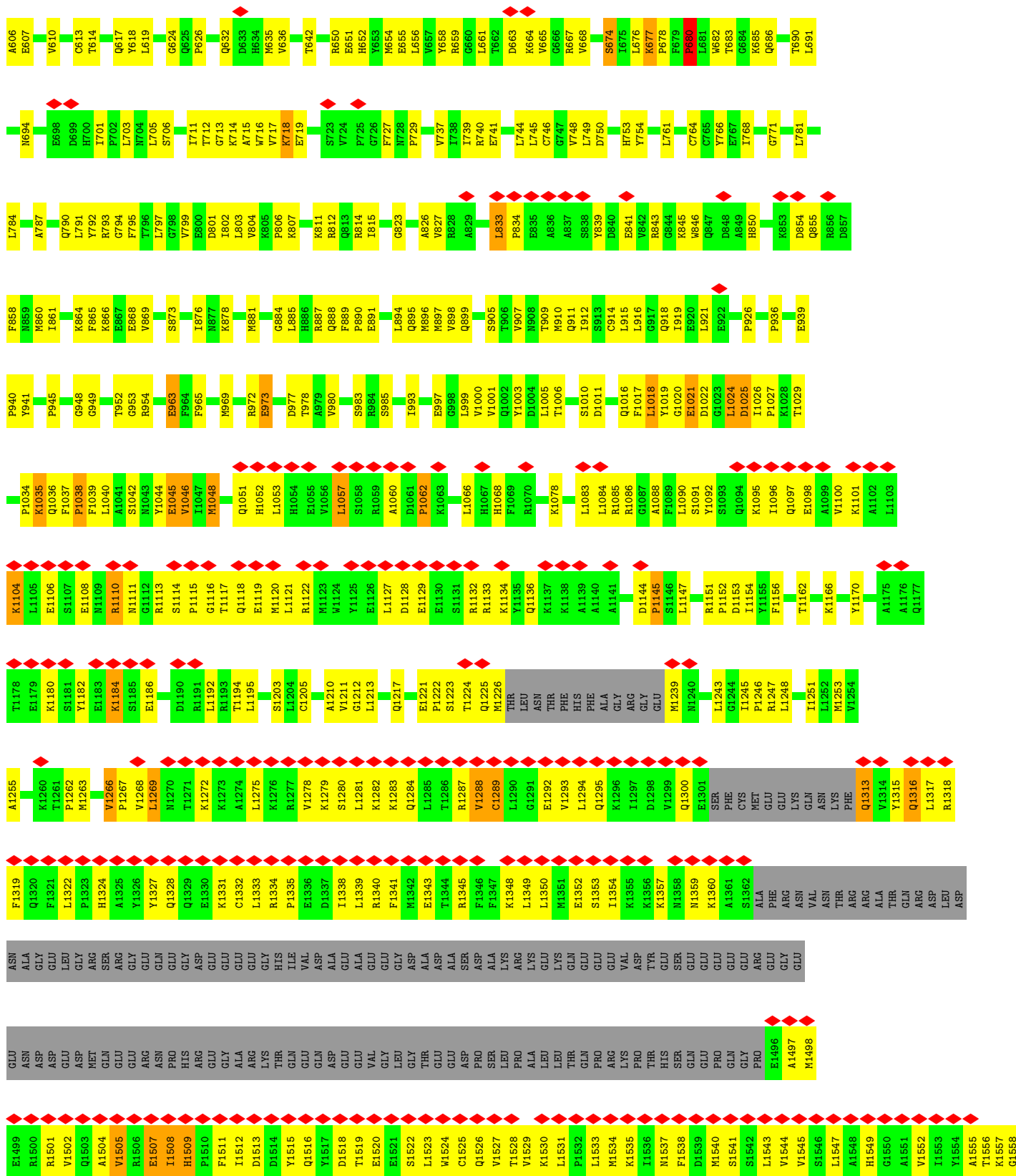
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

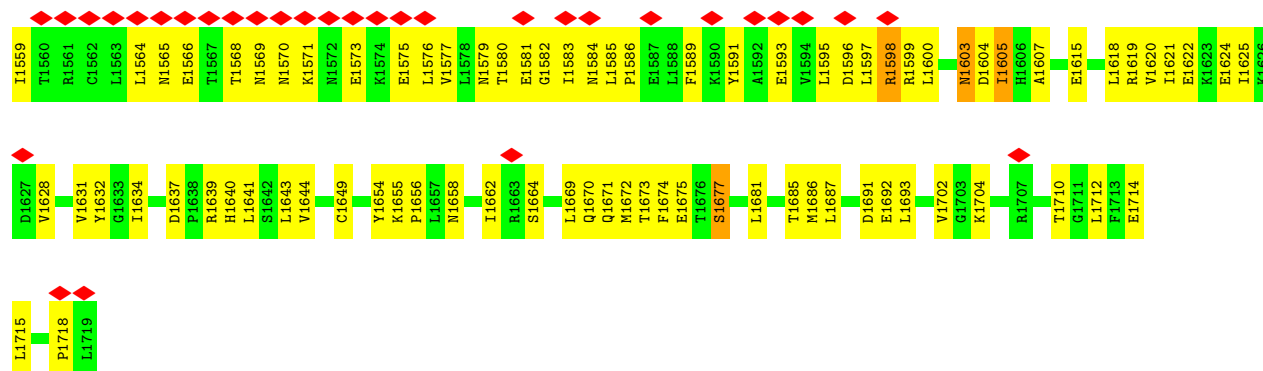
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

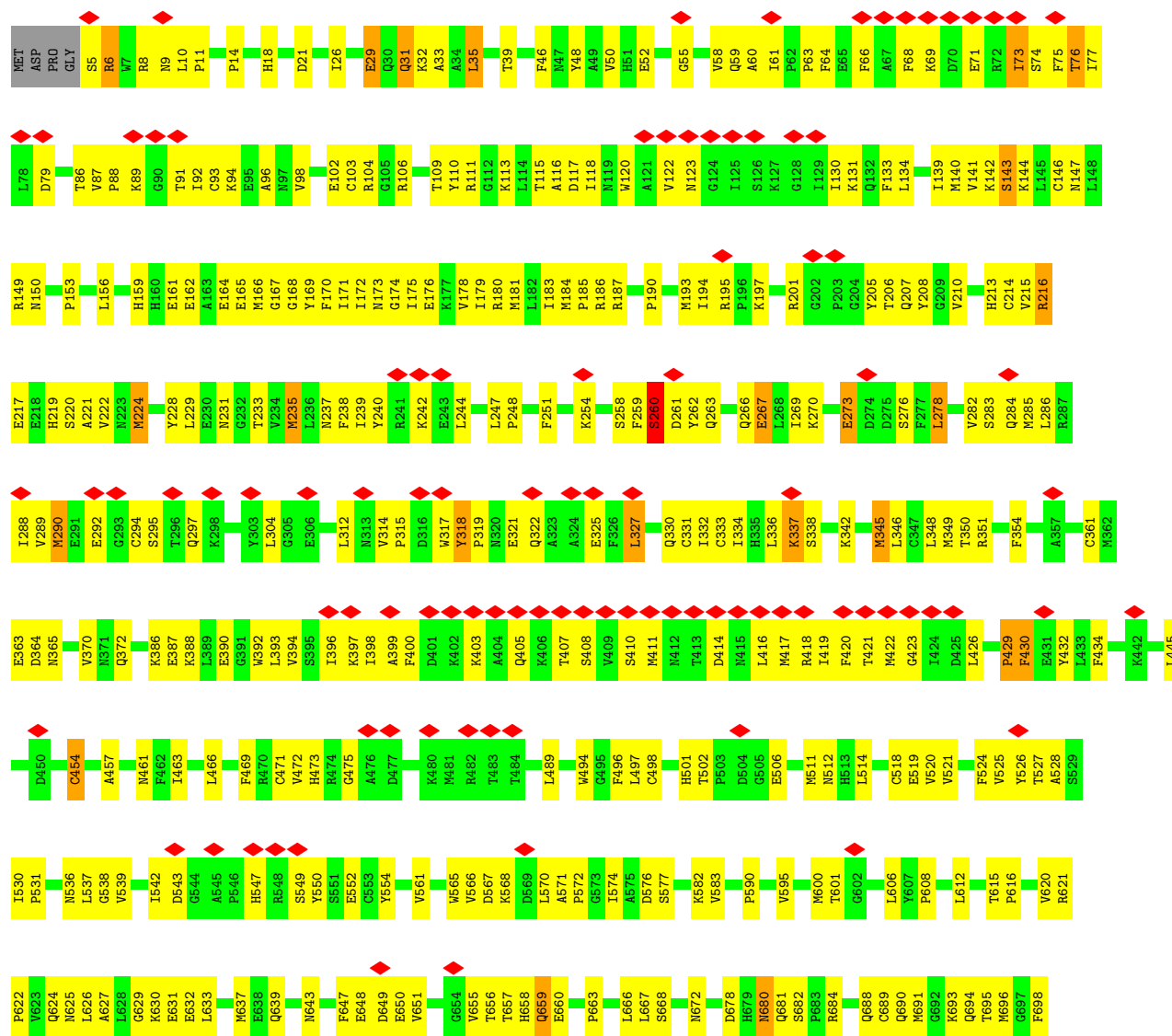


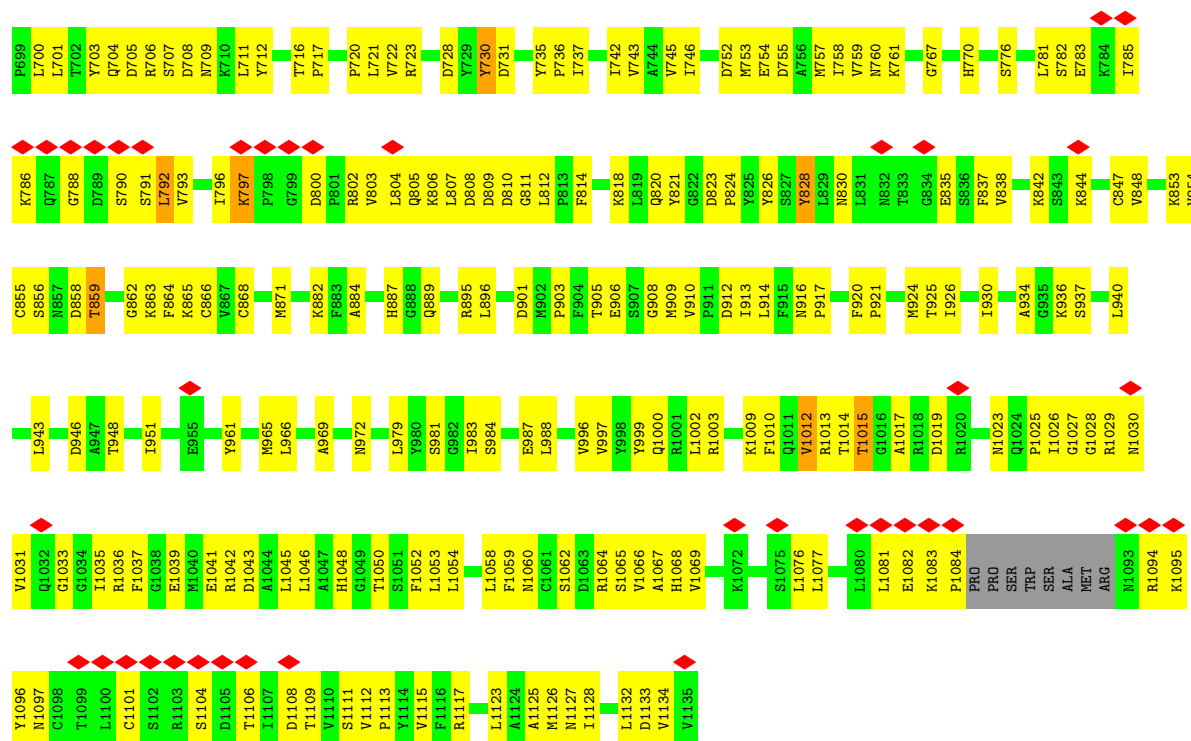




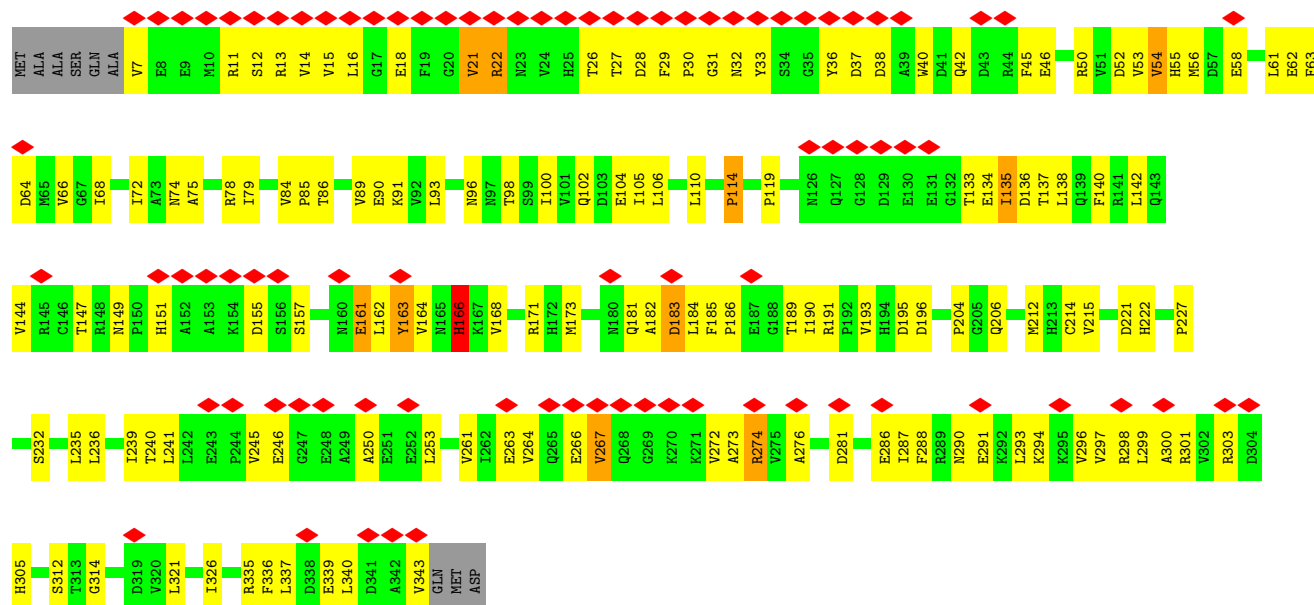


• Molecule 2: DNA-directed RNA polymerase I subunit RPA2



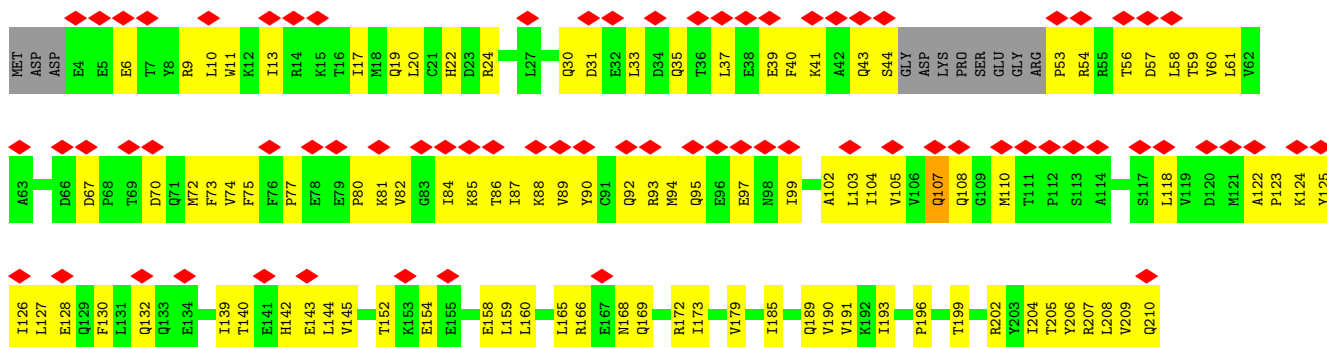


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

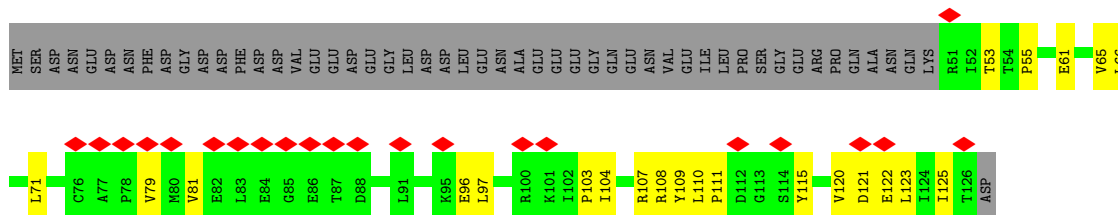


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

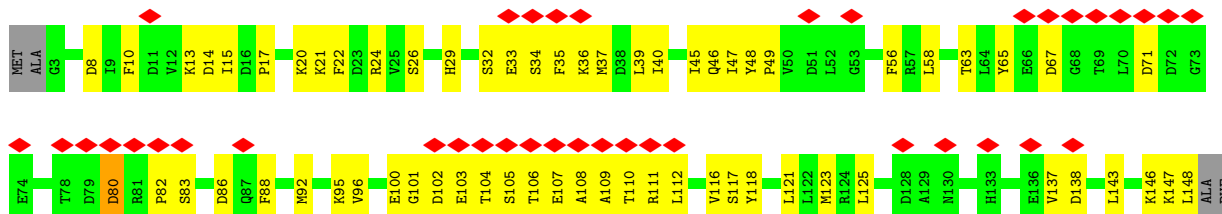




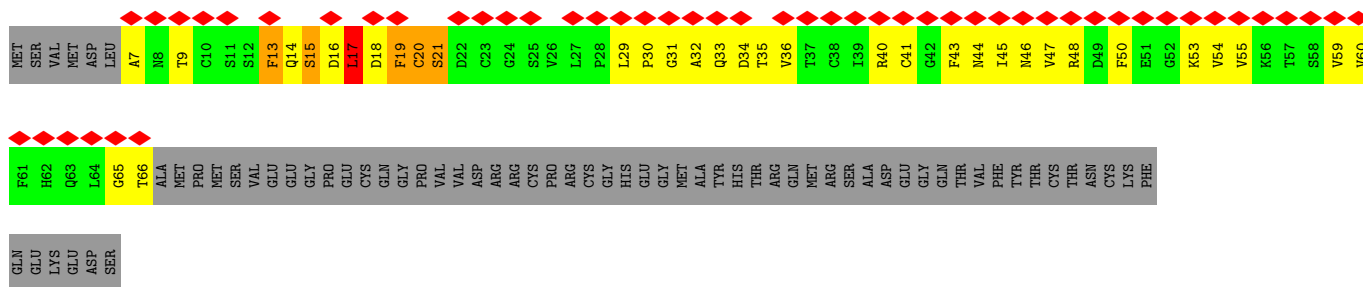
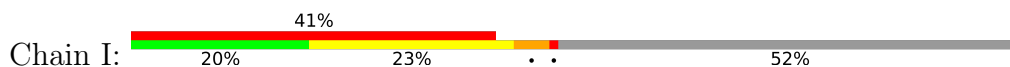
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

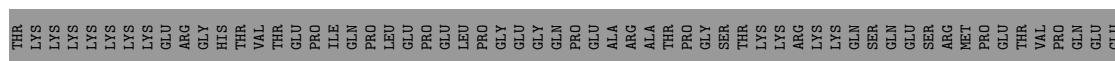


- Molecule 7: DNA-directed RNA polymerase I subunit RPA12

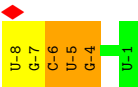


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5





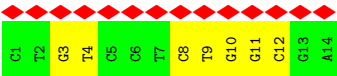




● Molecule 15: DNA (25-MER)



● Molecule 16: DNA (5'-D(\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*GP\*CP\*GP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.000	Depositor
Minimum map value	-3.528	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.687	Depositor
Map size ( $\text{\AA}$ )	334.08002, 334.08002, 334.08002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.044, 1.044, 1.044	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	2/11988 (0.0%)	0.73	9/16184 (0.1%)
2	B	0.51	4/9127 (0.0%)	0.76	8/12350 (0.1%)
3	C	0.50	0/2751	0.80	3/3729 (0.1%)
4	E	0.32	0/1669	0.49	0/2254
5	F	0.32	0/620	0.48	0/839
6	H	0.38	0/1197	0.60	1/1614 (0.1%)
7	I	0.84	1/454 (0.2%)	1.24	6/615 (1.0%)
8	J	0.47	0/516	0.83	1/696 (0.1%)
9	K	0.35	0/878	0.61	0/1182
10	L	0.33	0/385	0.55	0/511
11	N	0.76	2/1140 (0.2%)	0.87	2/1560 (0.1%)
12	G	0.33	0/1252	0.55	0/1691
13	M	0.69	0/884	0.79	2/1192 (0.2%)
14	R	0.36	0/186	0.92	0/287
15	T	0.65	0/579	0.84	1/892 (0.1%)
16	U	0.53	0/313	0.95	0/481
All	All	0.50	9/33939 (0.0%)	0.74	33/46077 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	20	CYS	C-N	15.33	1.69	1.34
11	N	57	ASN	C-N	6.47	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	38	PRO	N-CD	5.75	1.55	1.47
2	B	143	SER	CA-CB	-5.59	1.44	1.52
2	B	283	SER	CA-CB	-5.45	1.44	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	13	PHE	O-C-N	12.88	143.31	122.70
7	I	13	PHE	CA-C-N	-12.18	90.42	117.20
8	J	10	CYS	CB-CA-C	-11.81	86.78	110.40
7	I	20	CYS	O-C-N	-11.17	104.82	122.70
7	I	13	PHE	C-N-CA	-9.68	97.51	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	8	PHE	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11749	0	11888	723	0
2	B	8912	0	8896	563	0
3	C	2697	0	2676	158	0
4	E	1641	0	1671	106	0
5	F	610	0	642	18	0
6	H	1176	0	1137	54	0
7	I	447	0	429	72	0
8	J	507	0	523	26	0
9	K	863	0	850	69	0
10	L	379	0	387	23	0
11	N	1105	0	1098	47	0
12	G	1229	0	1212	0	0
13	M	867	0	844	67	0
14	R	168	0	85	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	T	514	0	279	40	0
16	U	281	0	160	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	33151	0	32777	1727	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 1727 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:SER:HB3	7:I:18:ASP:CB	1.44	1.45
7:I:20:CYS:C	7:I:21:SER:N	1.69	1.45
13:M:33:LEU:HD22	13:M:39:MET:CE	1.47	1.43
2:B:260:SER:CB	7:I:18:ASP:HB2	1.45	1.42
11:N:142:PRO:CG	11:N:145:LEU:HD21	1.50	1.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1455/1719 (85%)	1309 (90%)	137 (9%)	9 (1%)	25	54
2	B	1119/1135 (99%)	1019 (91%)	100 (9%)	0	100	100
3	C	335/346 (97%)	312 (93%)	23 (7%)	0	100	100
4	E	195/210 (93%)	185 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
6	H	144/150 (96%)	130 (90%)	14 (10%)	0	100	100
7	I	58/126 (46%)	41 (71%)	14 (24%)	3 (5%)	2	5
8	J	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
9	K	106/133 (80%)	96 (91%)	9 (8%)	1 (1%)	17	44
10	L	43/58 (74%)	37 (86%)	6 (14%)	0	100	100
11	N	149/510 (29%)	134 (90%)	13 (9%)	2 (1%)	12	34
12	G	153/338 (45%)	138 (90%)	14 (9%)	1 (1%)	22	51
13	M	108/419 (26%)	107 (99%)	1 (1%)	0	100	100
All	All	4001/5338 (75%)	3639 (91%)	346 (9%)	16 (0%)	38	64

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	1035	LYS
1	A	1605	ILE
7	I	21	SER
11	N	156	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1295/1503 (86%)	1205 (93%)	90 (7%)	15	40
2	B	982/992 (99%)	913 (93%)	69 (7%)	15	39
3	C	296/302 (98%)	274 (93%)	22 (7%)	13	36
4	E	183/192 (95%)	181 (99%)	2 (1%)	73	91
5	F	66/111 (60%)	66 (100%)	0	100	100
6	H	129/131 (98%)	126 (98%)	3 (2%)	50	80
7	I	53/111 (48%)	51 (96%)	2 (4%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	53/56 (95%)	50 (94%)	3 (6%)	20	49
9	K	96/119 (81%)	94 (98%)	2 (2%)	53	82
10	L	42/55 (76%)	41 (98%)	1 (2%)	49	80
11	N	119/427 (28%)	114 (96%)	5 (4%)	30	62
12	G	135/288 (47%)	132 (98%)	3 (2%)	52	81
13	M	94/366 (26%)	90 (96%)	4 (4%)	29	60
All	All	3543/4653 (76%)	3337 (94%)	206 (6%)	24	48

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	317	TRP
2	B	680	ASN
12	G	94	ASP
2	B	330	GLN
2	B	463	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	690	GLN
3	C	180	ASN
2	B	709	ASN
2	B	1068	HIS
4	E	132	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/8 (87%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	-6	C
14	R	-5	U
14	R	-4	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	20:CYS	C	21:SER	N	1.69

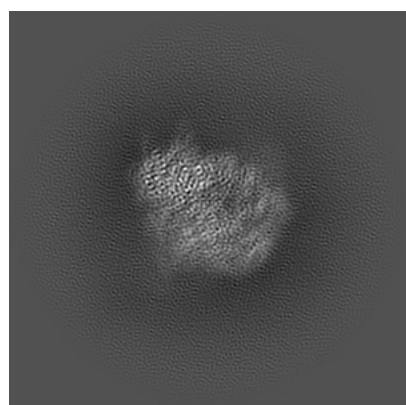
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31877. These allow visual inspection of the internal detail of the map and identification of artifacts.

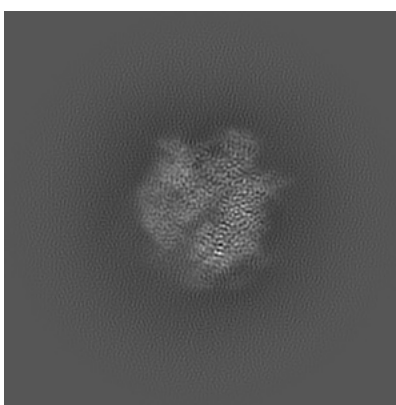
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

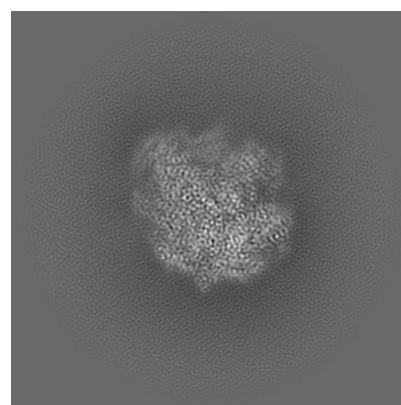
#### 6.1.1 Primary map



X



Y

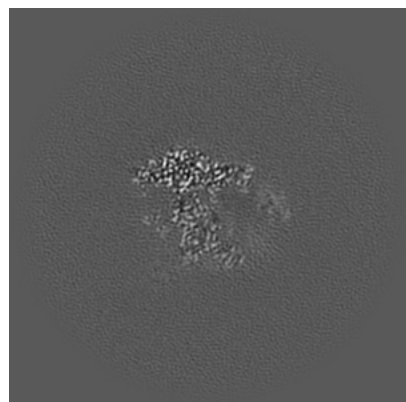


Z

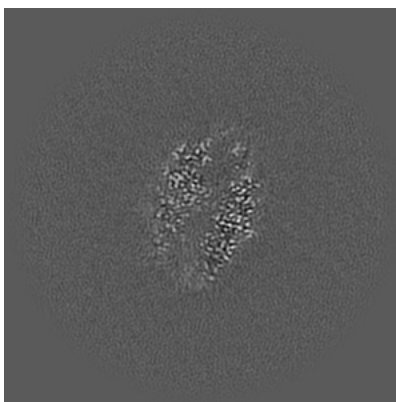
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

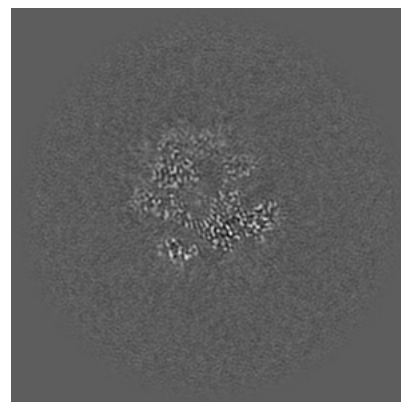
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

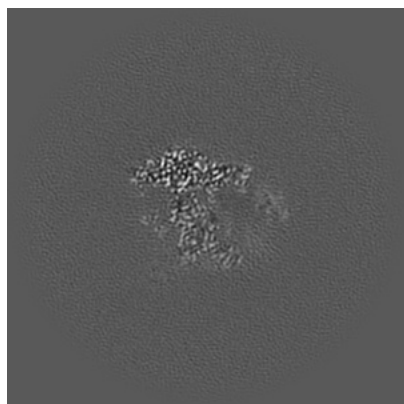


Z Index: 160

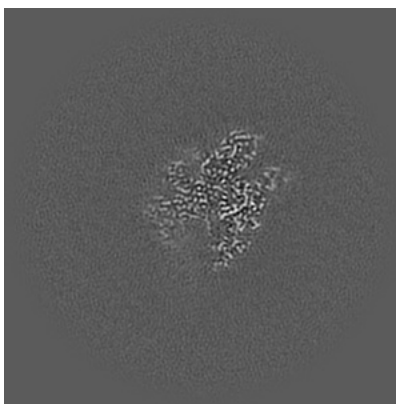
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

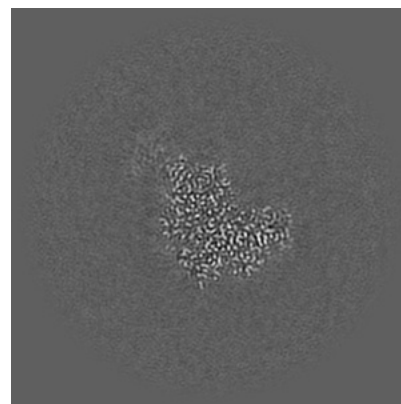
### 6.3.1 Primary map



X Index: 160



Y Index: 141

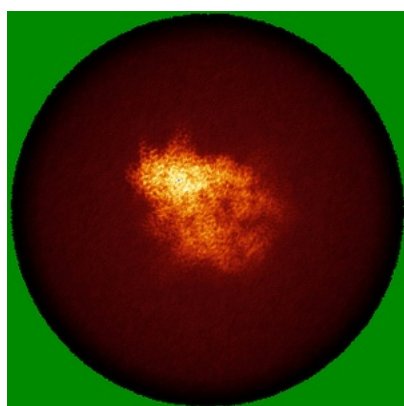


Z Index: 184

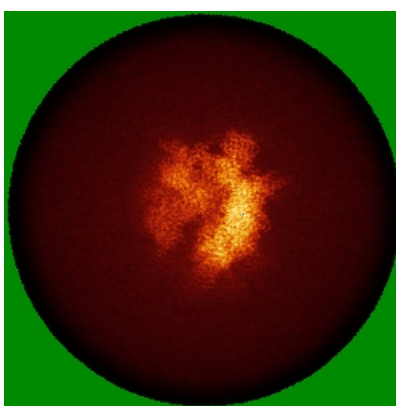
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

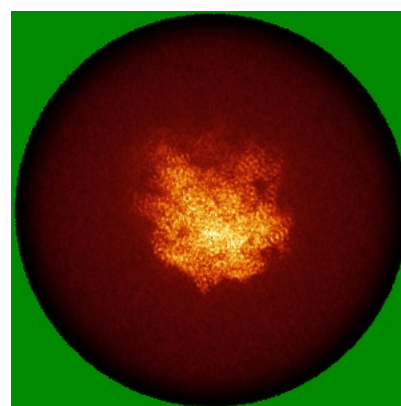
### 6.4.1 Primary map



X



Y

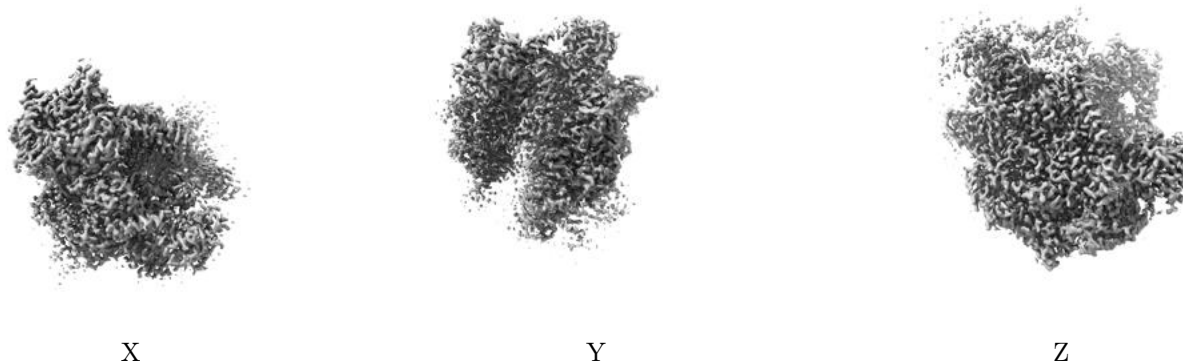


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.687. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

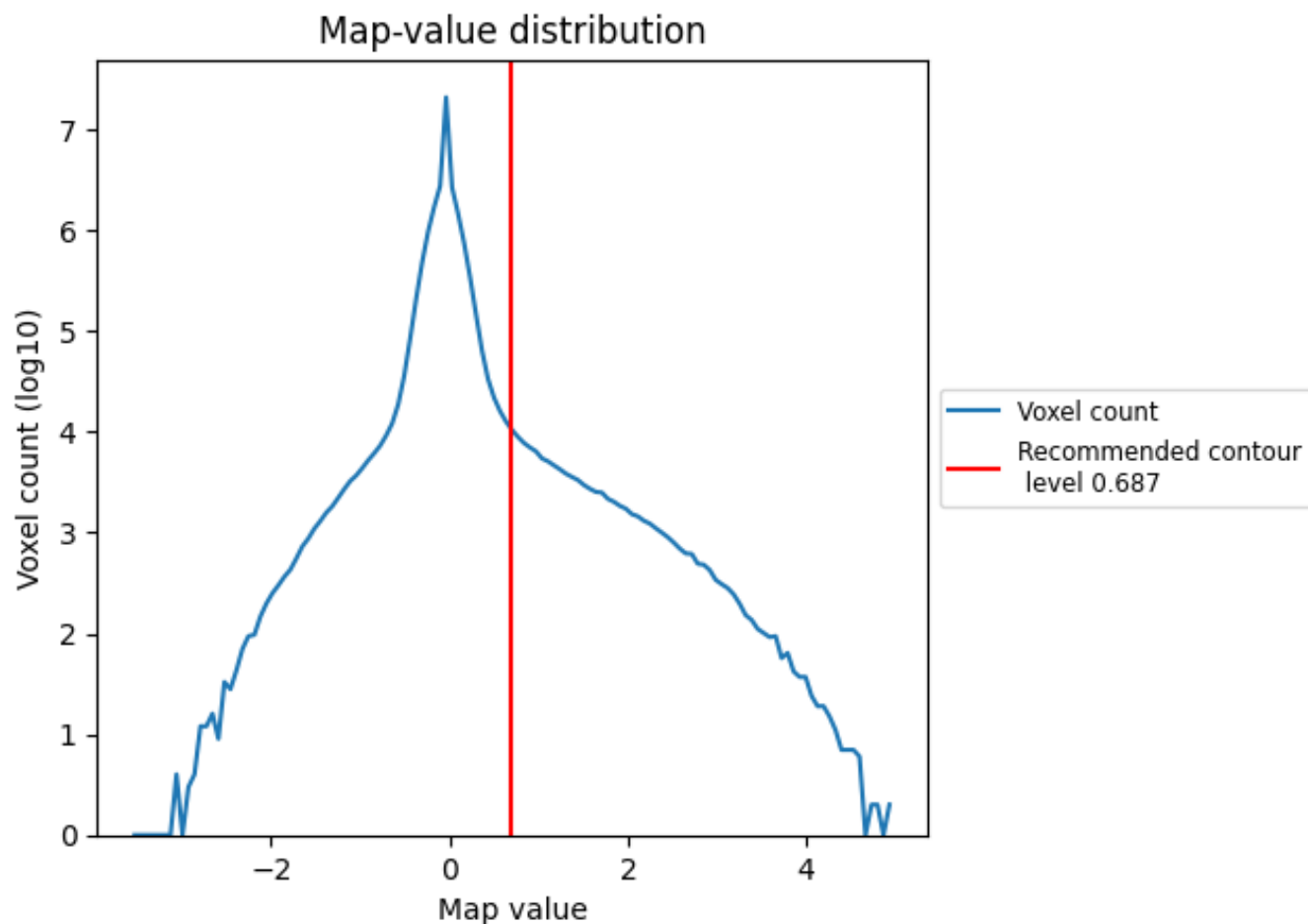
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

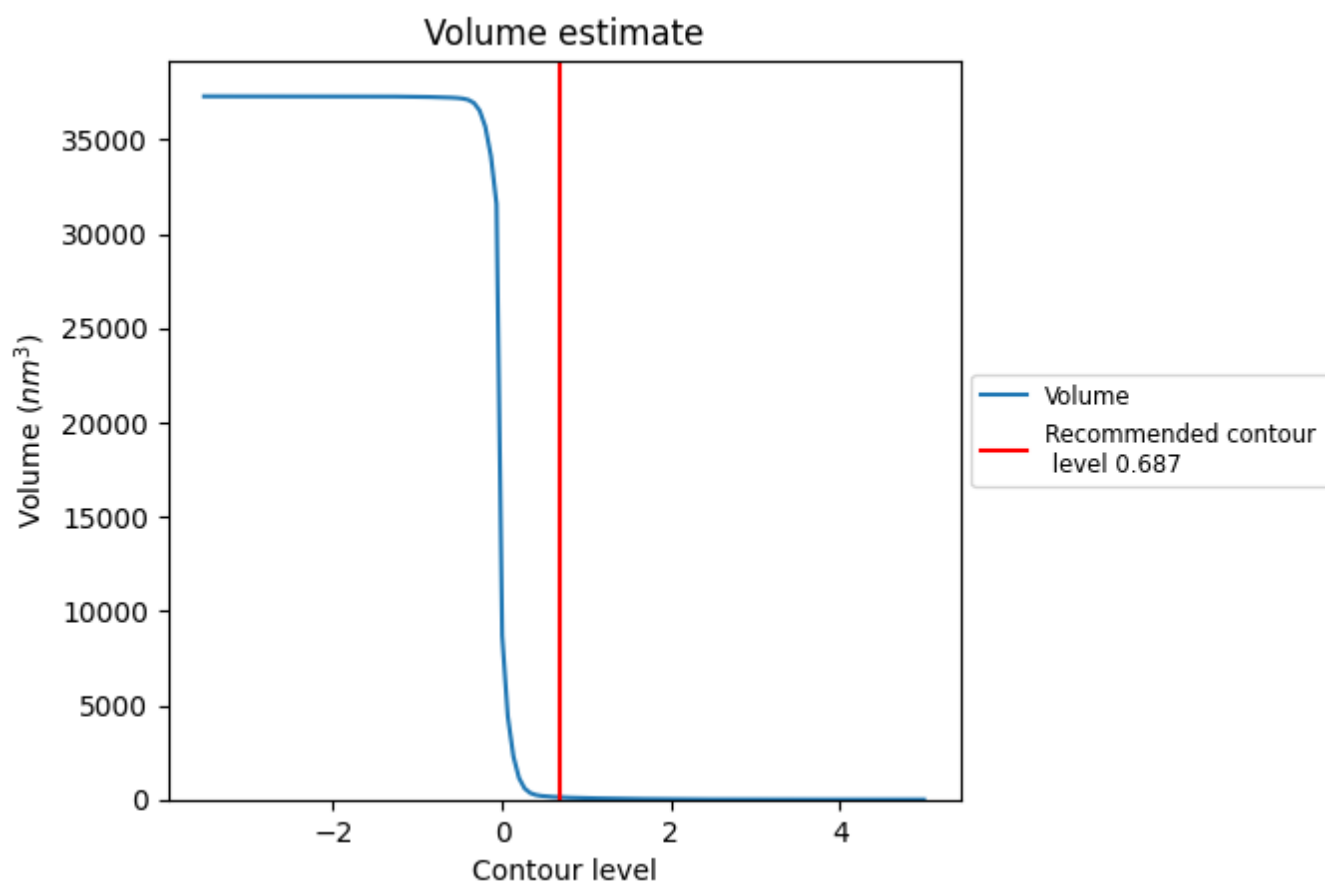
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

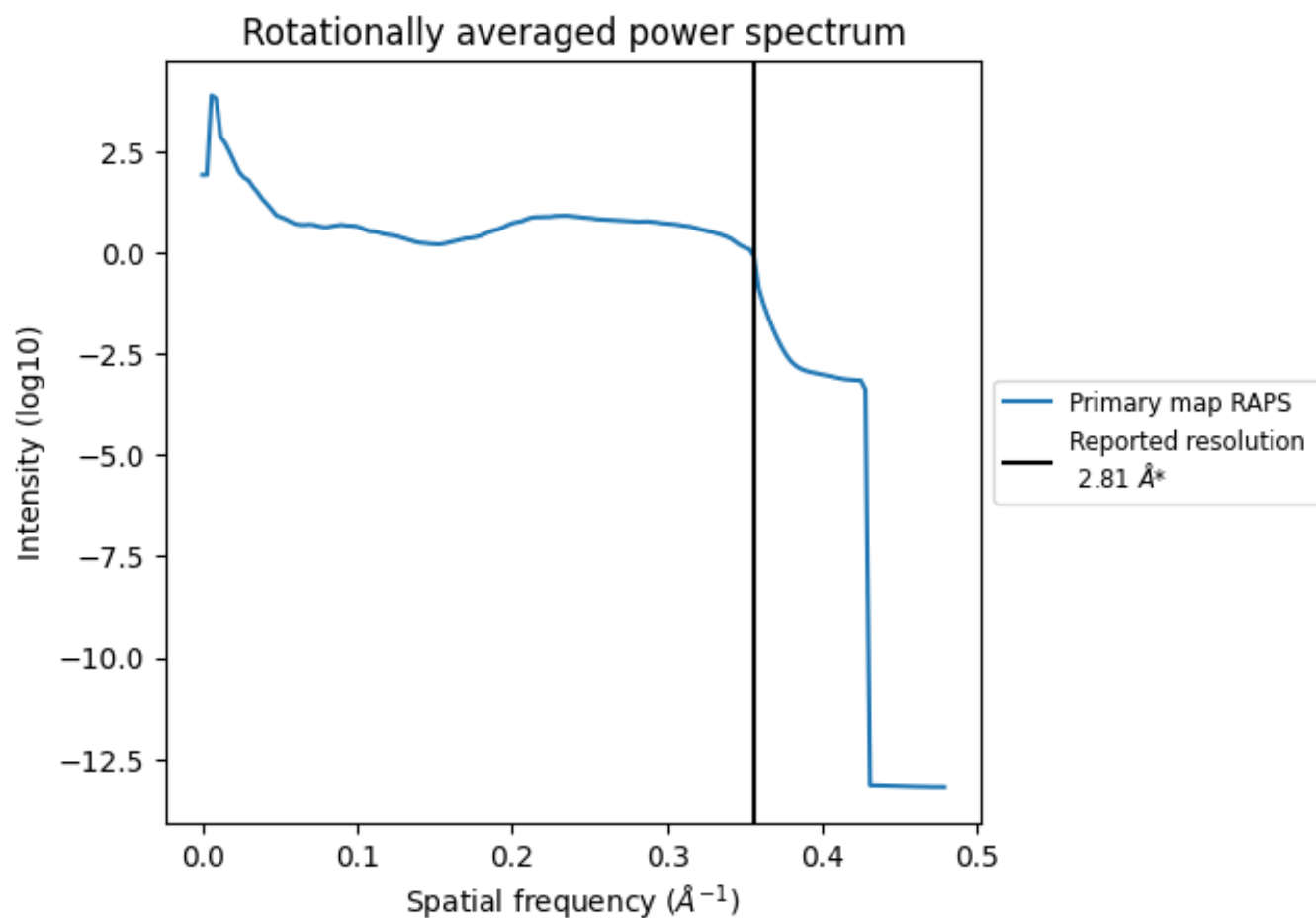
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122  $\text{nm}^3$ ; this corresponds to an approximate mass of 110 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.356 Å<sup>-1</sup>

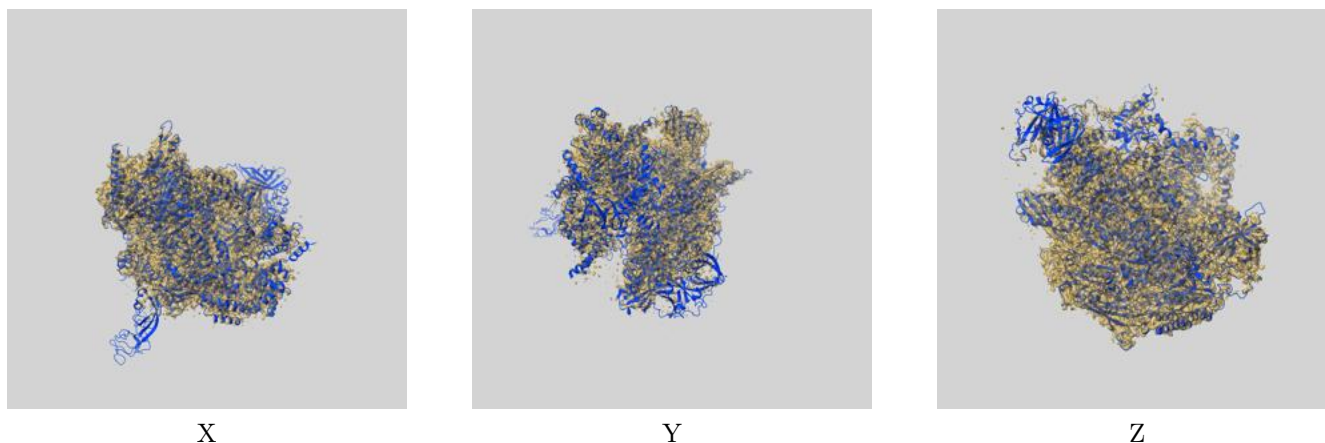
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

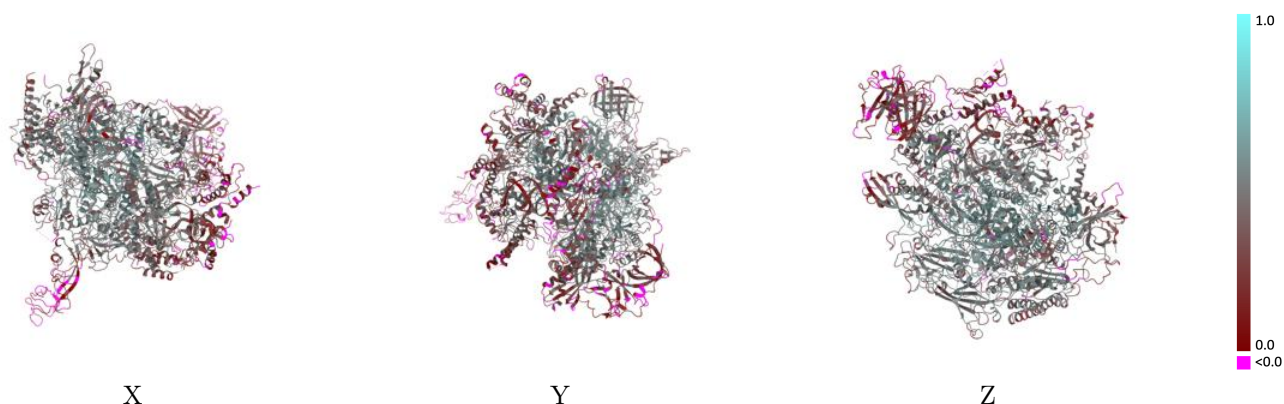
This section contains information regarding the fit between EMDB map EMD-31877 and PDB model 7VBB. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



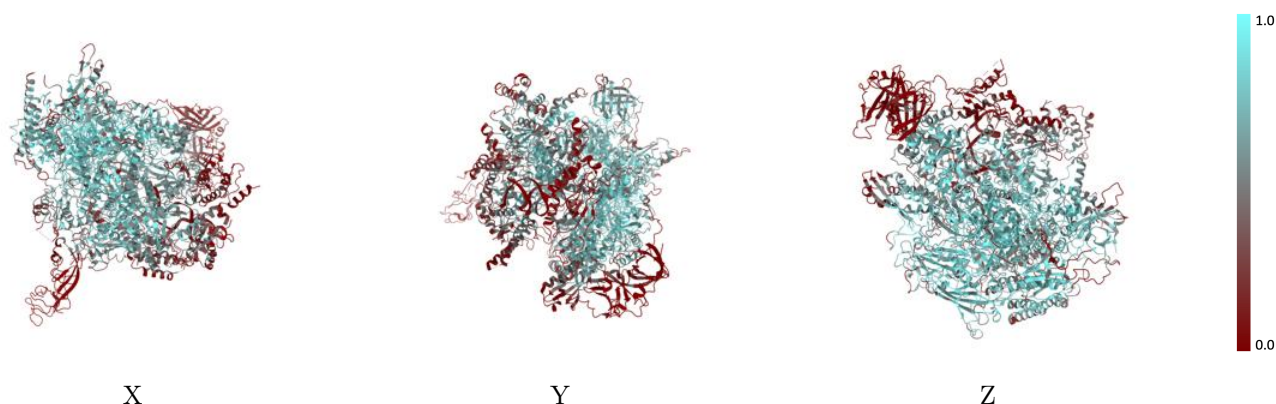
The images above show the 3D surface view of the map at the recommended contour level 0.687 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



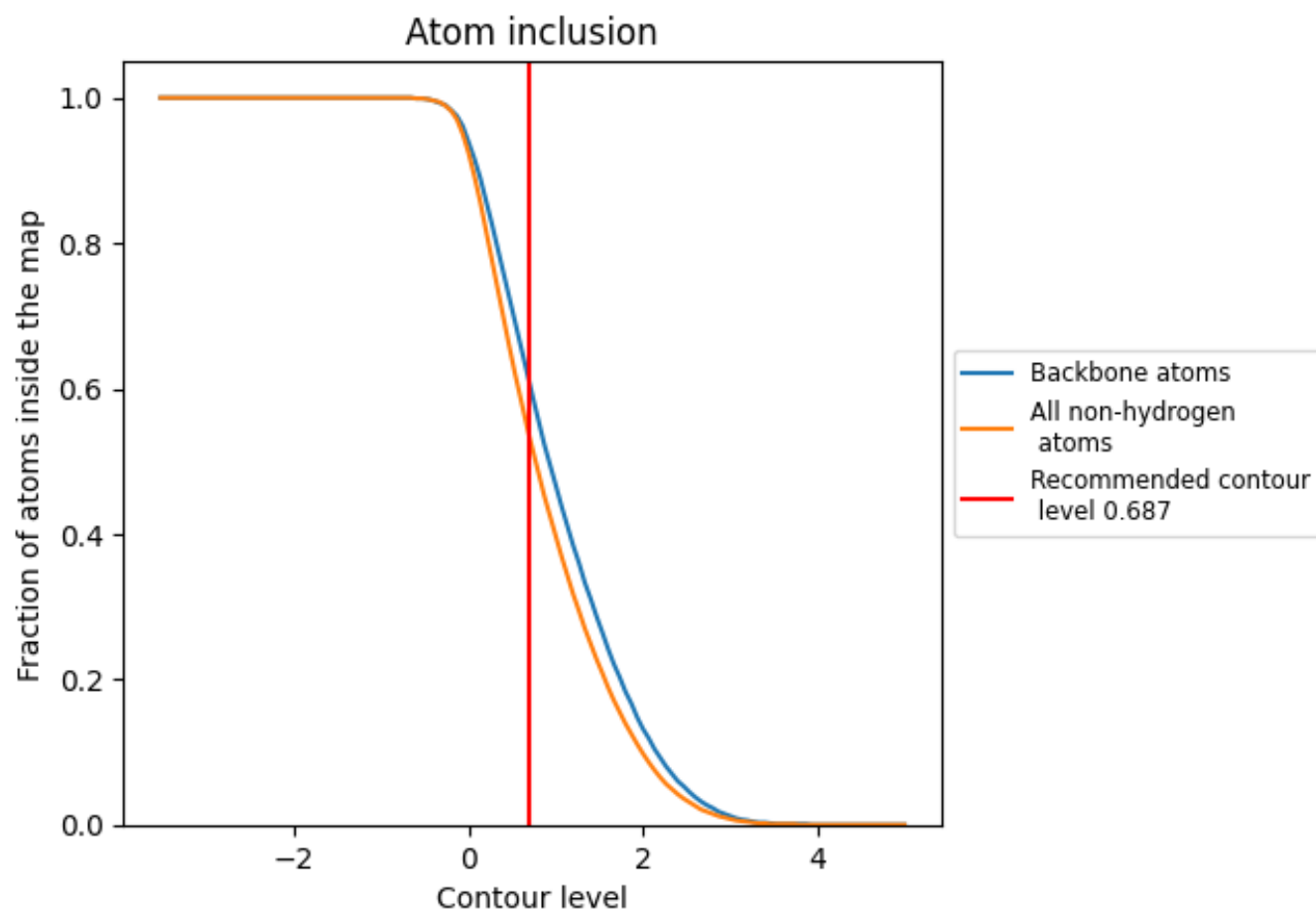
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.687).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.687) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5400	 0.4010
A	 0.5430	 0.4150
B	 0.6980	 0.4790
C	 0.6070	 0.4120
E	 0.5030	 0.3580
F	 0.5650	 0.4440
G	 0.0510	 0.1130
H	 0.5620	 0.3680
I	 0.1510	 0.1350
J	 0.8060	 0.5320
K	 0.6630	 0.4290
L	 0.7190	 0.4510
M	 0.0910	 0.1910
N	 0.0570	 0.1860
R	 0.6250	 0.5260
T	 0.3910	 0.3970
U	 0.0710	 0.2690

